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Bounds on Green's functions of second-order differential equations

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We estimate the diagonal part of the Green's function for the equation $(-\Delta/2 + V(x) + \partial/\partial t)\psi(x,t) = 0, t>0, x\in B$, where B is a finite region of the Euclidean space R^d with a regular boundary. In the special case $V(x) = 0$, $x\in B$, we also obtain bounds for the non-diagonal part of the Green's function which are uniform in t.

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I. INTRODUCTION

Kac, in unpublished lecture notes summarized in Ref. 1, indicates how Wiener estimates of the Green's function for the one-particle diffusion equation can be used to derive results about the bulk properties of the free boson gas. The mathematical details were supplied in Lewis and Pulè.[2] The same strategy has been used in van den Berg and Lewis[3] to prove results (announced in Ref. 4) about the boson gas in an external potential. For this purpose we require Wiener estimates of the Green's function for the one-particle diffusion equation with an external potential. These estimates may be of use in other fields of application and the purpose of this paper is to provide their proofs.

We estimate the Green's function of the partial differential equation

$$(L + \partial/\partial t)\psi(x,t) = 0, \quad x\in B,\ t>0, \tag{1}$$

where B is a finite region of the Euclidean space R^d with a regular boundary ∂B. We will restrict ourselves to Dirichlet boundary conditions: $\psi(x,t) = 0$ for $x\in\partial B$. L denotes the self-adjoint operator on the space $L^2(B)$ which is given on smooth functions by the differential operator $-\Delta/2 + V(x)$ with Dirichlet boundary conditions where $V(x)$ is a non-negative function (satisfying a Lipschitz condition almost everywhere in B). This operator has a discrete positive spectrum $E_1 < E_2 \leqslant E_3 \cdots$ and an orthonormal set of eigenfunctions $\{\phi_j(x)\}$ forming a basis in $L_2(B)$ (Davies[5]). Furthermore, the Green's function of (1) has the eigenfunction expansion

$$K(x,y;t) = \sum_{j=1}^{\infty} \exp(-tE_j)\phi_j(x)\phi_j(y). \tag{2}$$

Moreover, it has been shown by Rosenblatt[6] and Ray[7] that $K(x,y;t)$ can be written as

$$K(x,y;t) = \frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}} \times \mathrm{E}\left\{\exp\left[-\int_0^t V(u(\tau))d\tau\right]: u(0) = x,\ u(t) = y;\ u(\tau)\in B\right\}, \tag{3}$$

where the quantity

$$\mathrm{E}\left\{\exp\left[-\int_0^t V(u(\tau))d\tau\right]: u(0) = x,\ u(t) = y;\ u(\tau)\in B\right\}$$

denotes the average value of

$$\exp\left[-\int_0^t V(u(\tau))d\tau\right]$$

for all paths $u(\cdot)$ of a Wiener process on R^d subject to $u(0) = x$ and $u(t) = y$. Furthermore Ray[7] proved that $K(x,y;t)$ is continuous (for all y) at a point x_0 of the boundary ∂B provided there exists a conical sector with vertex at x_0 entirely outside B. We will assume that this condition holds for all points on the boundary; we call such a boundary regular. Ray[7] has, in addition, results in the case in which B is an unbounded region of R^d and $V(x)\to\infty$ as $|x|\to\infty$; we will restrict ourselves, however, to the case in which B is a bounded region.

Our main result is that for t small

$$K(x,x;t) \sim e^{-tV(x)}/(2\pi t)^{d/2} \tag{4}$$

at all points x which are not too close to the boundary. Expression (4) can easily be understood from formula (3). For small times t the probability is small that $|x - u(\tau)|$ is large, so we may replace $u(\tau)$ by x and B by R^d, provided x is not too close to ∂B. This has been called the principle of not feeling the boundary.[8] Integrating both sides of (4) with respect to the volume we have, for t small,

$$\sum_{j=1}^{\infty} \exp(-tE_j) \sim \frac{1}{(2\pi t)^{d/2}} \int_{x\in B} e^{-tV(x)}\, dx. \tag{5}$$

This is allowed, since most points x are far from the boundary because the boundary is regular.

In Sec. 2 we will estimate the Green's function of the differential equation (1) for the special case $V(x) = 0$, $x\in B$. In Secs. 3 and 4 we will calculate bounds on the correction terms in (4) and (5).

2. A UNIFORM ESTIMATE WHEN V IS IDENTICALLY ZERO

Theorem 1: Let $K_0(x,y;t)$ be the Green's function of Eq. (1) with $V(x) = 0$, $x\in B$, and with Dirichlet boundary conditions for $\psi(x,t)$ at ∂B.
Then

$$\left|K_0(x,y;t) - \frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\right| \leqslant \frac{2d}{(2\pi t)^{d/2}} \exp\left((4\sqrt{2} - 6)\frac{d_x^2}{dt}\right),\ x\in B,\ y\in B,\ t>0, \tag{6}$$

where d_x is the distance of x from ∂B.

Proof: Let $\square_x$ denote a hypercube with center x which lies entirely inside B and such that at least one corner vertex lies on ∂B. Then the length l_x of an edge of the cube is not less then $(2/d^{1/2})d_x$. From (3) we have

$$0\leqslant K_0(x,y;t)=\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\times\mathbb{E}\{1:u(0)=x,\,u(t)=y;\,u(\tau)\in B\}$$
$$\leqslant\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\,\mathbb{E}\{1:u(0)=x,\,u(t)=y;\,u(\tau)\in R^d\}$$
$$=\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}. \tag{7}$$

We consider two cases:

(i) $|x-y|\geqslant\alpha l_x$, where $\alpha\in[0,\frac12)$. (We will choose α later). In this case we have by (7) the bound

$$\left|K_0(x,y;t)-\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\right|\leqslant\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\leqslant\frac{\exp(-\alpha^2 l_x^2/2t)}{(2\pi t)^{d/2}}. \tag{8}$$

(ii) $|x-y|\leqslant\alpha l_x$, where $\alpha\in[0,\frac12)$. It is obvious that $y\in\square_x$ since $\alpha\leqslant\frac12$. Because of the inequality (7) we have only to derive a lower bound for $K_0(x,y;t)$

$$K_0(x,y;t)\geqslant\frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}\times\mathbb{E}\{1:u(0)=x,\,u(t)=y;\,u(\tau)\in\square_x\}. \tag{9}$$

Denote the right-hand side of (9) by $K_\square(x,y;t)$; $K_\square(x,y;t)$ is the Green's function for a cube with edges with lengths l_x and center x. We have the following explicit expression if we choose x as the origin and the rectangular coordinate frame parallel to the edges of the cube:

$$K_\square(0,y;t)=\prod_{i=1}^{d}\left(\frac{1}{l_x}\sum_{k=-\infty}^{+\infty}\exp\left[-\frac{\pi^2 t}{2l_x^2}(2k+1)^2\right]\cos\frac{(2k+1)\pi y_i}{l_x}\right).$$

With the help of the Poisson formula[9] we obtain

$$K_\square(0,y;t)=\prod_{i=1}^{d}\frac{\exp(-y_i^2/2t)}{(2\pi t)^{\frac12}}\times\left\{1+2\sum_{k=1}^{\infty}(-)^k\exp\left(-\frac{k^2l_x^2}{2t}\right)\cosh\frac{ky_il_x}{t}\right\}.$$

The terms of the alternating series in k are decreasing provided $|y_i|<l_x/2$. The term $k=1$ is negative so the sum is also negative but larger than or equal to -1, since the Green's function is non-negative. With the use of

$$\prod_{i=1}^{d}(1+a_i)\geqslant 1+\sum_{i=1}^{d}a_i,\quad -1\leqslant a_i\leqslant 0,\ d=1,2\cdots$$

we have

$$K_\square(x,y;t)\geqslant\frac{\exp(-y^2/2t)}{(2\pi t)^{d/2}}\times\left[1+2\sum_{i=1}^{d}\sum_{k=1}^{\infty}(-)^k\exp\left(-\frac{k^2l_x^2}{2t}\right)\cosh\frac{ky_il_x}{t}\right]$$
$$\geqslant\frac{\exp(-y^2/2t)}{(2\pi t)^{d/2}}\left[1-2\sum_{i=1}^{d}\exp\left(-\frac{l_x^2}{2t}\right)\cosh\frac{y_il_x}{t}\right]$$
$$\geqslant\frac{\exp(-y^2/2t)}{(2\pi t)^{d/2}}\left[1-2\sum_{i=1}^{d}\exp\left(-\frac{l_x^2}{2t}+\frac{|y_i|l_x}{t}\right)\right]$$
$$\geqslant\frac{\exp(-y^2/2t)}{(2\pi t)^{d/2}}\left[1-2d\exp\left(-\frac{l_x^2}{t}(\tfrac12-\alpha)\right)\right], \tag{10}$$

since $|y|\leqslant\alpha l_x$. Now, we choose α to be the positive root of $\frac12-\alpha=\alpha^2/2$. So $\alpha=-1+\sqrt{2}$, which is also less than $\frac12$. Combining the results (7), (8), and (9) we arrive at Theorem 1.

If $x=y$ we may choose $\alpha=0$ and we have

$$\left|K_0(x,x;t)-\frac{1}{(2\pi t)^{d/2}}\right|\leqslant\frac{2d}{(2\pi t)^{d/2}}\exp\left(-\frac{2d_x^2}{dt}\right), \tag{11}$$

which is a stronger inequality than one would obtain from Theorem 1 by putting $x=y$. Notice that Theorem 1 is a stronger result than that of Arima[10] since it is uniform in t. On the other hand we have obtained it only in the case of Dirichlet boundary conditions.

3. THE MAIN ESTIMATE

Theorem 2: Let B be a finite region in R^d with a regular boundary ∂B and let $V(x)$ be a non-negative Borel-measurable function defined on B. Let $V(x)$ satisty a local Lipschitz condition of the form

$$|V(x)-V(x')|<M(x)\cdot|x-x'|^\alpha,\quad 0<\alpha\leqslant1$$

for almost all pairs x, x' in B; then

$$\left|\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}-K(x,x;t)\right|$$
$$\leqslant\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\left\{2d\exp\left(-\frac{2d_x^2}{dt}\right)+\left|\int_0^t d\tau\int_{u\in B}du\,(V(u)-V(x))\left(\frac{t}{2\pi\tau(t-\tau)}\right)^{d/2}\exp\left(-\frac{t|x-u|^2}{2\tau(t-\tau)}\right)\right|\right.$$
$$\left.+\left|\int_0^t\frac{d\tau}{t}\int_{u\in B}du\left(\frac{t}{2\pi\tau(t-\tau)}\right)^{d/2}\exp\left(t(V(x)-V(u))-\frac{t|x-u|^2}{2\tau(t-\tau)}\right)-1\right|\right\}, \tag{12}$$

at all points x where the Lipschitz condition holds.

Proof: From the theorems of Ray[7] and Rosenblatt[6] it follows that

$$\frac{e^{-tV(x)}}{(2\pi t)^{d/2}} - K(x,x;t) = \frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big\{\mathbb{E}\Big\{1-\exp\Big[-\int_0^t [V(u(\tau))-V(x)]\,d\tau\Big]:u(0)=u(t)=x;u(\tau)\in B\Big\}$$
$$+1-\mathbb{E}\{1:u(0)=u(t)=x;u(\tau)\in B\}\Big\}$$
$$\leqslant \frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big\{\mathbb{E}\Big\{\int_0^t [V(u(\tau))-V(x)]d\tau:u(0)=u(t)=x;u(\tau)\in B\Big\}$$
$$+2d\exp\Big(-\frac{2d_x^2}{dt}\Big)\Big\} = \frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big\{\int_0^t d\tau\int_{u\in B} du\,(V(u)-V(x))\cdot\Big(\frac{t}{2\pi t(t-\tau)}\Big)^{d/2}\exp\Big(-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)$$
$$+2d\exp\Big(-\frac{2d_x^2}{dt}\Big)\Big\}\leqslant\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big\{\Big|\int_0^t d\tau\int_{u\in B} du\,(V(u)-V(x))$$
$$\cdot\Big(\frac{t}{2\pi t(t-\tau)}\Big)^{d/2}\exp\Big(-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\Big| + 2d\exp\Big(-\frac{2d_x^2}{dt}\Big)\Big\}, \tag{13}$$

by the inequality $1-e^{-x}\leqslant x$, Theorem 1, and Fubini's theorem. Moreover

$$K(x,x;t) = \frac{1}{(2\pi t)^{d/2}}\mathbb{E}\Big\{\exp\Big[-\int_0^t V(u(\tau))\,d\tau\Big]:u(0)=u(t)=x;u(\tau)\in B\Big\}$$
$$\leqslant\frac{1}{(2\pi t)^{d/2}}\mathbb{E}\Big\{\int_0^t\frac{d\tau}{t}\,e^{-tV(u(\tau))}:u(0)=u(t)=x;u(\tau)\in B\Big\}$$
$$\leqslant\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\int_0^t\frac{d\tau}{t}\int_{u\in B}\exp\Big(-t(V(u)-V(x))-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\Big(\frac{t}{2\pi\tau(t-\tau)}\Big)^{d/2}, \tag{14}$$

by Jensen's inequality and Fubini's theorem. Combining (13) and (14) we have estimate (12).

4. AN ESTIMATE FOR THE PARTITION FUNCTION

In this section we estimate the correction term in (5). This can be done by simply integrating the inequalities (13) and (14) from which an estimate follows. However, due to an inequality of Ray[7] the result can be improved.

Theorem 3: Let $V(x)$ and B be as in Theorem 2, then

$$\Big|\sum_{j=1}^{\infty}\exp(-tE_j)-\int_{x\in B}dx\,\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big|\leqslant\frac{1}{(2\pi t)^{d/2}}\int_{x\in B}dx\cdot e^{-tV(x)}\Big\{2d\exp(-2d_x^2/dt)$$
$$+\Big|\int_0^t d\tau\int_{u\in B}du\,(V(u)-V(x))\exp\Big(-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\cdot\Big(\frac{t}{2\pi\tau(t-\tau)}\Big)^{d/2}\Big|\Big\}. \tag{15}$$

Proof: We first prove an upper bound (Ray[7]).

$$\sum_{j=1}^{\infty}\exp(-tE_j)$$
$$=\int_{x\in B}K(x,x;t)dx\leqslant\frac{1}{(2\pi t)^{d/2}}\int_{x\in B}dx\int_0^t\frac{d\tau}{t}\,\mathbb{E}\{e^{-tV(u(\tau))}:u(0)=u(t)=x;u(\tau)\in B\}$$
$$=\frac{1}{(2\pi t)^{d/2}}\int_{x\in B}dx\int_0^t\frac{d\tau}{t}\int_{u\in B}du\cdot\exp\Big(-tV(u)-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\cdot\Big(\frac{t}{(2\pi\tau)(t-\tau)}\Big)^{d/2}$$
$$\leqslant\frac{1}{(2\pi t)^{d/2}}\int_{x\in R^d}dx\int_0^t\frac{d\tau}{t}\int_{u\in B}du\,\exp\Big(-tV(u)-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\cdot\Big(\frac{t}{(2\pi\tau)(t-\tau)}\Big)^{d/2}$$
$$=\frac{1}{(2\pi t)^{d/2}}\int_{u\in B}e^{-tV(u)}du, \tag{16}$$

by Jensen's inequality. Moreover it follows from (13) that

$$\int_{x\in B}dx\Big(K(x,x;t)-\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big)\geqslant-\int_{x\in B}dx\,\frac{e^{-tV(x)}}{(2\pi t)^{d/2}}\Big\{\Big|\int_0^t d\tau\int_{u\in B}du\,(V(u)-V(x))\Big(\frac{t}{2\pi\tau(t-\tau)}\Big)^{d/2}$$
$$\cdot\exp\Big(-\frac{t|x-u|^2}{2\tau(t-\tau)}\Big)\Big|+2d\exp\Big(-\frac{2d_x^2}{dt}\Big)\Big\}. \tag{17}$$

Combining the bounds (16) and (17) we arrive at (15).

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